DOCKET NO.: 195832US0DIV

Marked-Up Copy

Serial No: 09/656,435

Amendment Filed on: 07/31/02

IN THE CLAIMS

Please amend claims 6-11 to read as follows:

--6. (Amended) A method <u>for determining stable ligand-biopolymer docking</u> <u>structures comprising</u> [which comprises]:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type or covalent bonds and three-dimensional coordinates for each atom of a ligand; wherein dummy atoms are preset at positions of heteroatoms that can hydrogen-bond with hydrogen bonding groups in the biopolymer;

covering possible docking structures between said biopolymer and said ligand while changing the conformation of said ligand; wherein matching of distances among dummy atoms and those among heteroatoms of the ligand are tested; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable one relative to the biopolymer; as well as the stability of said docking structures, the binding modes and conformations of the ligand in said structures[, wherein matching of distances among dummy atoms and those among heteroatoms of the ligand are tested, said dummy atoms being preset at the positions of the heteroatoms that can hydrogen-bond with hydrogen bonding groups in the biopolymer].

7. (Amended) A method for determining stable ligand-biopolymer docking structures

comprising [which comprises]:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type of covalent bonds and three-dimensional coordinates for each atom of a ligand; wherein dummy atoms are preset at the positions of heteroatoms that can hydrogen-bond with hydrogen-bonding groups in the biopolymer;

selecting [possible] <u>stable</u> docking structures between said biopolymer and said ligand while changing the conformation of said ligand; <u>wherein matching of distances among</u> <u>dummy atoms and those among heteroatoms of the ligand are tested;</u> and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable one relative to the biopolymer, as well as the stability of said docking structures, the binding modes and conformations of the ligand in said structures[, wherein matching of distances among dummy atoms and those among heteroatoms of the ligand are tested, said dummy atoms being preset at the positions of heteroatoms that can hydrogen-bond with hydrogen-bonding groups in the biopolymer].

8. (Amended) A method <u>for determining stable ligand-biopolymer docking structures</u>
<u>comprising</u> [which comprises]:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type of covalent bonds and three-dimensional coordinates for each atom of a ligand, wherein dummy atoms are preset at positions of atoms that can specifically interact with functional groups in the biopolymer;

covering possible docking structures between said biopolymer and said ligand while changing the conformation of said ligand, wherein matching of distances among dummy atoms and those among atoms of the ligand are tested; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable one relative to the biopolymer, as well as the stability of said docking strutures, the binding modes and conformations of the ligand in said structures[, wherein matching of distances among dummy atoms and those among atomes of the ligand are tested, said dummy atoms being preset at the positions of atoms that can specifically interact with functional groups in the biopolymer].

9. (Amended) A method <u>for determining stable ligand-biopolymer docking structures</u> <u>comprising</u> [which comprises]:

inputting three-dimensional coordinates for each atom of a biopolymer as well as atomic element, bond-type of covalent bonds and three-dimensional coordinates for each atom of a ligand, wherein dummy atoms are preset at positions of atoms that can specifically interact with functional groups in the biopolymer;

selecting [possible] <u>stable</u> docking structures between said biopolymer and said ligand while changing the conformation of said ligand, <u>wherein matching of distances among</u> dummy atoms and those among atoms of the ligand are tested; and

outputting information about three-dimensional coordinates for each atom of the ligand in one or more stable docking structures including the most stable one relative to the biopolymer, as well as the stability of said docking structures, the binding modes and conformations of the ligand in said structures[, wherein matching of distances among dummy atoms and those among atoms of the ligand are tested, said dummy atoms being preset at the positions of atoms that can specifically interact with functional groups in the biopolymer].

10. (Amended) A method for estimating stable docking structures between a biopolymer and a ligand, [wherein possible] comprising selecting stable docking structures [are selected] by matching of distances among dummy atoms and those among heteroatoms

of the ligand, said dummy atoms being preset at the positions of heteroatoms of the ligand that can be hydrogen-bonded with hydrogen bonding groups in the biopolymer.

11. (Amended) A method for estimating stable docking structures between a biopolymer and a ligand, [wherein possible] comprising selecting stable docking structures [are selected] by matching of distances among dummy atoms and those among atoms of the ligand, said dummy atoms being preset at the positions of atoms of the ligand that can specifically interact with functional groups in the biopolymer, while changing the conformation of the ligand.--

IN THE ABSTRACT

Applicants provide herewith the Abstract that was inadvertently not received by the Examiner in the previous response. Its entry in place of the original Abstract is respectfully requested.